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ADP013388

TITLE: Simulation Modelling of Ecological Appearance

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TITLE: Chemical and Biological Medical Treatment Symposium - Industry II World Congress on Chemical and Biological Terrorism

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18. SIMULATION MODELLING OF ECOLOGICAL APPEARANCE

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Ecological processes that are happening in the nature are under strong influence of human act and behaviour (consciously or no consciously), having great consequences for different eco-systems. Transforming the fitted discontinuous distributions to continuous solves the problem of modelling the continuous processes, for which the observed values were measured in discontinuous time periods. One of asymmetric threats today is a terrorist act by which the terrorist (s) can contaminate the origin of the drinking water. Waters are in ecological point of view the most harmful and vulnerable, but also the most important part of the Global eco-system. On the planet Earth, land makes 29.2, and water 70.8 percent. There are 1.38 billions cubic kilometers of water, out of which 97.4 percent is salt water, and 2.6 percent fresh water; out of this, only 3 percent is potable water. The aim of this work is modelling of ecological appearance with the special emphasize to the water purification. Using the simulation modelling methods and techniques, matched for discontinuous processes, the efficiency of different absorbing materials (active carbon, zeolite A, zeolite ZSM-5, TMAZ) that can be used with different pollutants (dibutyl sulphide. different arsenic substances, different organophosphorus substances). With all collecting data it is possible to predict use of these materials in the accidents and in the situations of terrorist acts. To control the entering parameters and to get the output simulation method we used one of the standard packages for discrete simulation, Service model v4.2 (ProModel Corporation, while for continuous control of the processes we used Extend v4 (Imagine That, Inc.).

Water

1. Liquid without colour, smell or taste that falls as rain, is in lakes and seas, and is used for drinking, washing etc.
2. This liquid is supplied to homes, factories etc. in pipes
3. A mass of this liquid, esp. a lake, a river, sea etc. (Oxford English Dictionary).

INTRODUCTION

The effective dissemination of CB agents is generally considered to be more difficult than their manufacture. For example, the popular scenario involving the poisoning of the water supply of a major metropolitan area does not appear very feasible, given the large quantities of agent that would be required and various filtering or purification measures usually in place. On the other hand, the water supply for a discrete installation could be vulnerable, as would be air conditioning systems of even quite large public buildings or tunnel networks, such as subways. Similarly, domed sports stadiums have been described as "ideal" targets for a terrorist CB attack intended to kill tens of thousands of people.

Acquisition of CB materials

- A wide range of potentially deadly chemical and biological (CB) agents, including various insecticides, industrial chemicals and potent toxins such as ricin, may be relatively easy to produce or otherwise acquire.
- Some deadly pathogens can be obtained by mail from scientific supply houses; in other cases it is possible to harvest them from nature or to "grow your own" with relatively unsophisticated equipment and limited expertise.

- It may be possible to steal deadly agents from civilian research facilities or military stockpiles. Nor is it inconceivable that a state sponsor of terrorism would be deliberately wiling to provide terrorists with CB weapons or materials, if it could convince itself of "plausible deniability" while using a surrogate group to inflict a devastating blow on an enemy.
- However, the manufacture of modern, weapons-grade nerve agents by terrorists themselves may not be easy as often assumed: it requires a sophisticated laboratory infrastructure due to thc use of high temperatures and the generation of corrosive and dangerous by-products.
- On the other hand, chemical blister agents, such as sulphur mustard, nitrogen mustard, and lewisite can be manufactured with little to moderate difficulty, although the acquisition of large quantities of the necessary precursors could arouse suspicious.
- As for biological agents, the principle obstacle is the development of a genuinely lethal strain in sufficient quantities to cause mass casualties.

What is softer than water?
What is harder than rock?
Still, soft water carves hard rock.
(Ovidius)

As already mentioned, ecological appearances are processes that are happening in the Nature under the great influence of human behavior (conscious or unconscious), which is the cause of the drastic consequences for them.

Although the processes are going continually, their course is not writing in continuity. Instead of that it is measured the state of their characteristics in the specific time. One of the asymmetric threats today also include the terroristic act by the source of potable water can be contaminated.

Waters are in ecological view the most jeopardized and the most loaded, but also the most important part of the global eco system.

On June 18, 1992 it was seen a lot of dead fishes in the river Bednja near village Stažnjevec. Nor far from that place is the drain channel of the sewage system of the town Ivanec. (Figure 1. Map of the place where the event happened)

After the water analyses it was confirmed that in water was found high concentration of cyanides, in the average value of 0.424 mg/L.

All around and downstream the river, in the distance of 5 km flora and fauna were destroyed.

That event was the target for us to try to investigate and find out the best apsorbing materials that can be used as ecological filters.

Modelling:

The digital process model for the simulation of absorption of paraoxon (as well as DBS and CN) on activated charcoal, ZA, SiO2, TMAZ, ZSM-5 and A12O3 are shown on the picture.

For every material for absorption, it is defined the specific rules about absorption of paraoxon (or other agents) through the **model Equation**, in which it is written the rule/ the possibility for the absorption of every specific material.

To make "the real" picture of the process of the absorption, for every material, we count the influence (dependence) of the absorption through the time (which is specific for every absorbing material), as the entering process.

This is fulfilled with the model for gendering the values by the process of accidental numbers through the **"best fitted distribution"**.

In this model we used **empirical distributions**. As the started value of the simulation experiment, started values of the concentration of paradoxes (an other agents) in water are taken.

This value is a constant.

These constant and generic values of the dependence of absorbance in time are the entering parameters for the simulation model which transform through the Equation to the output values of the concentration of paraoxon (DBS, KCN).

EXPERIMENTAL

Zeolites (ZA, Klinoptilolite (TMAZ)), and some other materials as SiO_2 and Al_2O_3 (because they are precursors in the synthesis of zeolites), and activated charcoal (already used as the absorbing material in some personal decontamination kits) were used as absorbents for the KCN.

To study the process of absorption of KCN on ZA, TMAZ, SiO_2, Al_2O_3 and charcoal 2 g of solid (5, 7.5 and 10 g) were put into the reaction vessel containing 25 ml of KCN solution (0.02 M) in water.

The moment the solid was added to the solution was taken as the zero time of absorption (t_{ab}= 0).

At various times after the process of absorption of KCN started (1, 2, 5, 10, 20, 30, 40 60, 120 min), suspension were drawn of for analysis, and centrifuged.
After that the tytrimetric reaction with $AgNO_3$ was used to calculated the concentration of absorbed KCN on different absorbing materials.

RESULTS AND DISCUSSION

Figure 2 shows the absorption of KCN on ZA, TMAZ, SiO_2, Al_2O_3 and charcoal (10g); a) concentration on absorbents, b) concentration in solutions.

With ZA it is not possible to absorb more than 50 % of starting concentration of KCN. With 2 g of ZA in first ten minutes, it is absorbed about 40 % of the starting concentration of KCN.

Using 5.0 g there is no great difference in maximum absorption of KCN. But, instead 5 min, in first two minutes it is reached the maximum of absorption, after which it is reached the plateau.

This plateau is for 5.0 g of ZA 45 %, and for 7.5 and 10.0 g 50 %.

Using klinoptilolite (TMAZ) the difference between use of 2.0 g or 10.0 g is in the time necessary to reach the plateau of absorption.

With 2.0 g, in first 5 minutes 40 % of the amount of KCN is absorbed. while in next 20-25 minutes it is reached the maximum of absorption.

Using 5.0, 7.5 and 10.0 g the time in which the plateau is reached is moved to the left. In first 5 minutes absorption of KCN using 5.0 g of TMAZ is 48 %, using 7.5 g 55 %, and using 10.0 g amount 65 %.

Using alumina for absorption of KCN there is no big difference when it is used 2.0, 5.0, 7.5 or 10.0 g.

The maximum is reached after 30 minutes and using alumina it is possible to absorb more than 55 % of initiated amount of KCN.

The use of silica and charcoal shows similar characteristics (Fig. 3 a, b and Fig 4 a,b). With silica (Fig. 3. a, b), even with only 2.0 g, it is possible to have the same characteristics as with the use of 10.0 g.

With charcoal, there is the difference in the time reaching the plateau (Fig. 4 a, b).

With 2.0 g, after 5 minutes the absorption of KCN is about 50 %, with 5.0 g and 7.5 g about 65 % and with 10.0 g 80 %, what is almost the maximum amount of absorbing KCN.

The maximum for 5.0 g and 7.5 g is reached after 20 min, and for 2.0 g after an hour.

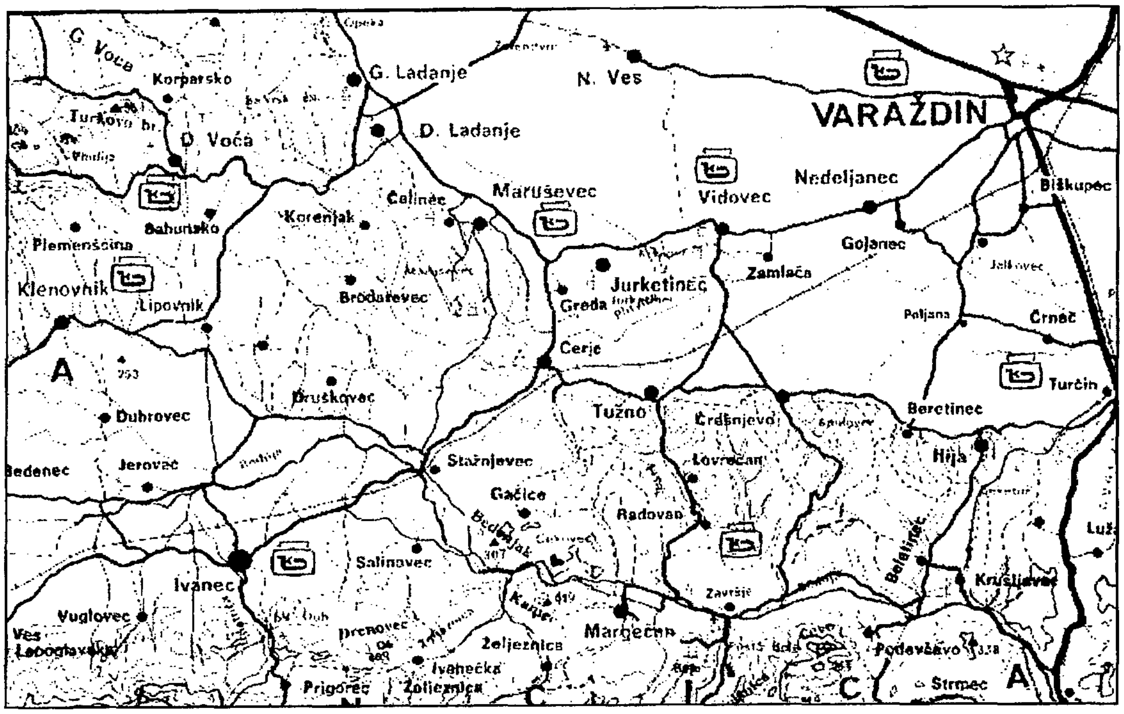
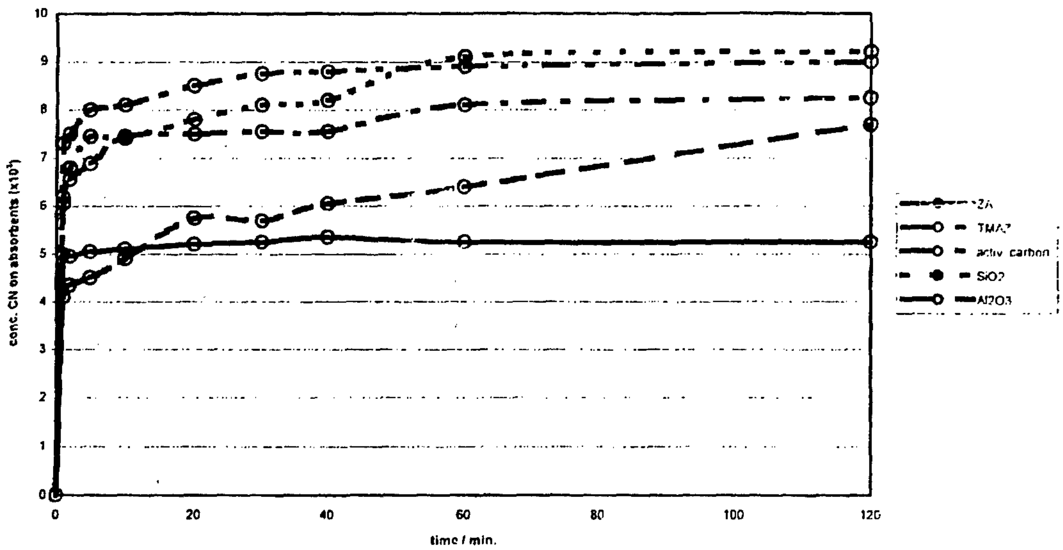
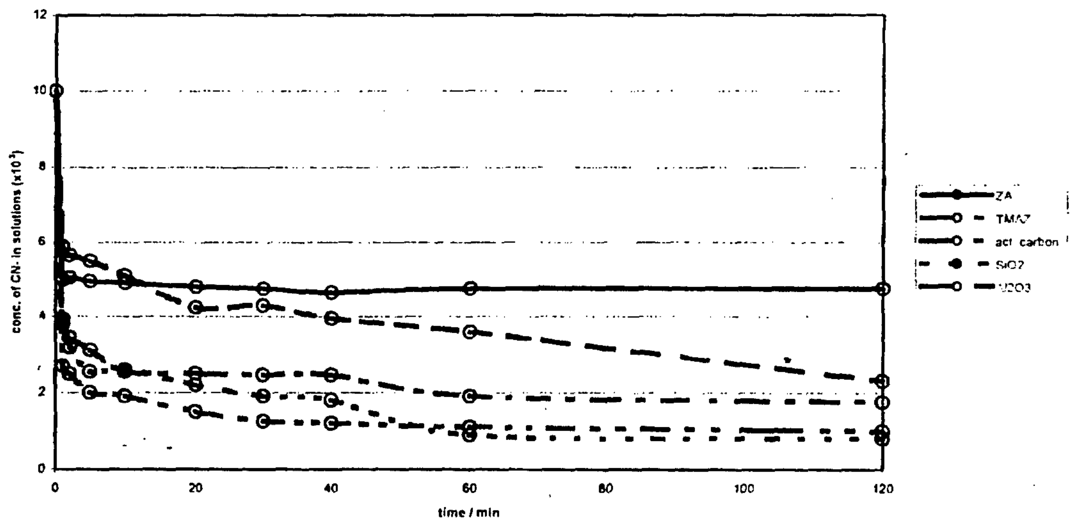


Figure 1. Map of the region and the place where the event happened.

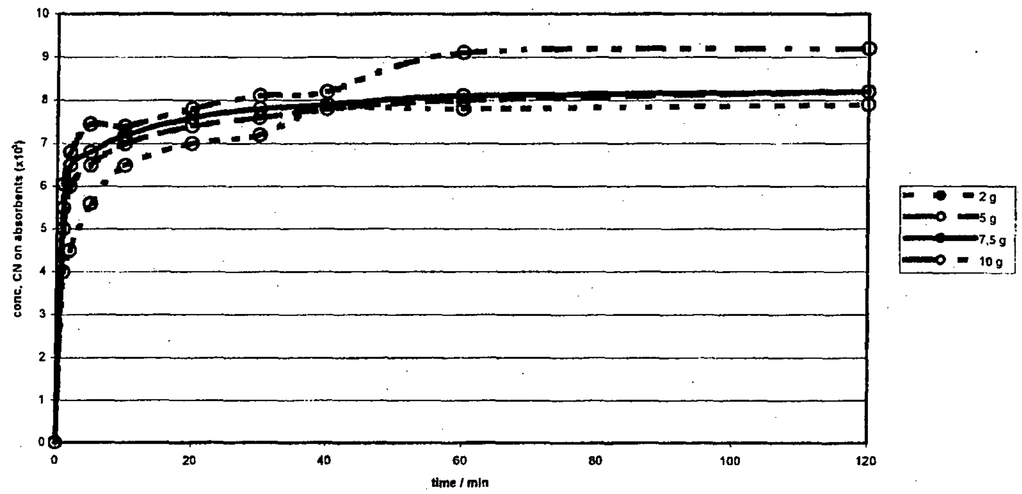


a)



b)

Figure 2. The absorption of KCN on ZA, TMAZ, SiO_2, Al_2O_3 and charcoal (10g); a) concentration of KCN on absorbents, b) concentration in solutions.



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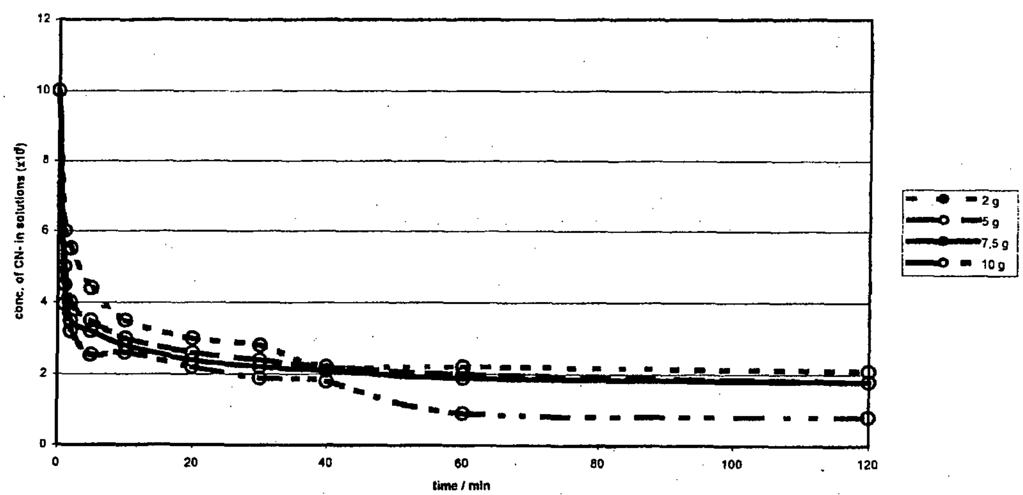
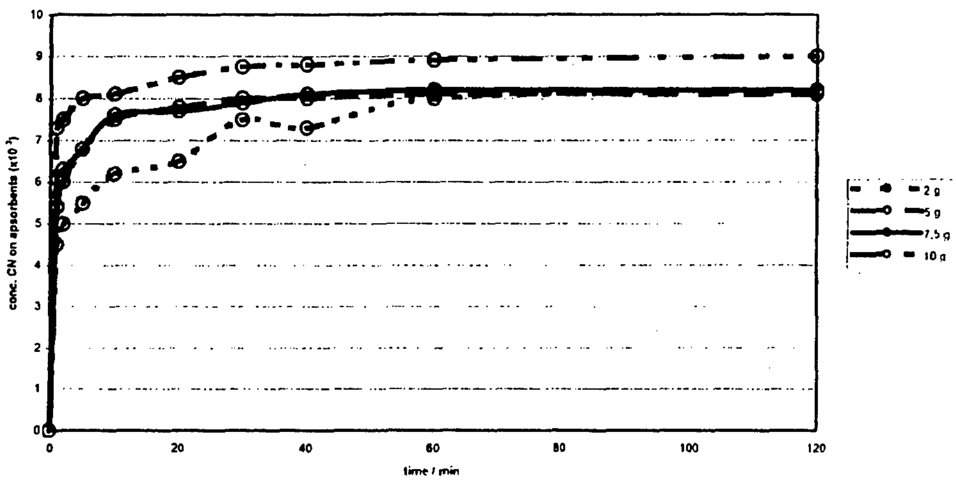


b)

Figure 3. Absorption of KCN on SiO_2 (2.0; 5.0; 7.5 and 10.0 g).
a) concentration of KCN on absorbent b) concentration in solution



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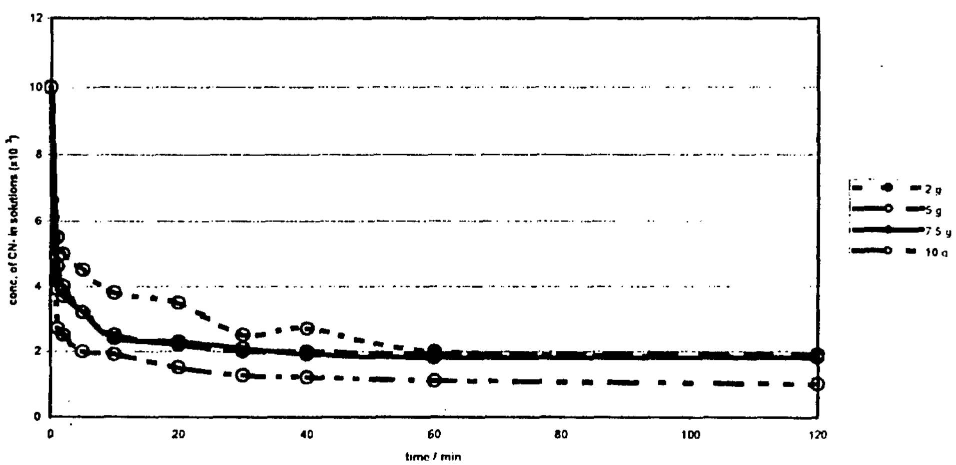

b)

Figure 4. Absorption of KCN on charcoal (2.0; 5.0; 7.5 and 10.0 g).
a) concentration of KCN on absorbent b) concentration in solution

CONCLUSIONS:

- There is great difference in absorption of KCN in different materials (ZA, TMAZ, activated charcoal, SiO_2, Al_2O_3)
- Using 2.0 g of absorbing material efficiency falls down in order $ZA < TMAZ < Al_2O_3 <$ activated carbon $< SiO_2$. The same order can be seen using 10.0 g of absorbing material.
- For ZA with 2.0 g of ZA the absorbing maximum is reached after 8-10 minutes and it is about 40 % of the initial concentration of KCN.
- For 5.0, 7.5 and 10.0 g the absorbing maximum is reached in 2-5 minutes, and it is between 45 and 50 % of the initial concentration of KCN.
- For other absorbing materials there is no great difference in use of different amount of absorbency (especially for 2.0, 5.0 and 7.5 g) and absorbing maximum is reached after 5 minutes. Taking into consideration all mentioned above, all the materials could be used as the absorbing materials in the kit for personal decontamination. Based on these results it seemed that the best results could be achieved with silica. Probably, even better results can be achieved with silica fumed, because of the available surface.
- About the model, after the model is made, its evaluation must confirm the possibility of its use in the real system. Evaluation is confirmed with statistical tests (hi square Kolmogorov- Smirnov test or Anderson- Darling test). Using this model it can be predicted in any time the concentration of the chemical agent in the solution and the amount of the agent that is absorbed. Comparing all adsorbents, it is possible to get the information which absorbing material is the most efficient. Beside that, the simulation experiments can be done even for the chemical agents for whom experimental adsorption measurements were not done.
- Also, it can be predict the most useful combination of adsorbing materials (in percentage).

KEY WORDS
Asymmetric threats, modelling, active carbon, zeolites

REFERENCES

1. G. R. Alther, Waste Management, 15 (8), (1995) 623.
2. R. Cintoli, B. Di Sabatino, L. Galeotti, G. Bruno, Wat. Sci. Tech., 32 (12) (1995) 73.
3. A. Čižmek, Suplement to the Proceedings from the 6th CBW Protection Symposium, Stockholm, Sweden (1998) 232.
4. A. Čižmek, Suplement to the Proceedings from the 6th CBW Protection Symposium, Stockholm, Sweden (1998) 233.
5. A. Čižmek, XVI. Hrvatski skup kemičara i kemijskih inženjera, Split 1999, Abstracts I, 324.
6. V. Strahonja, M. Varga, M. Pavlić, Projektiranje informacijskih sustava, Hrvatska informatička zajednica Zagreb i INA- industrija nafte, INFO Zagreb, Zagreb, (1992.) 108.